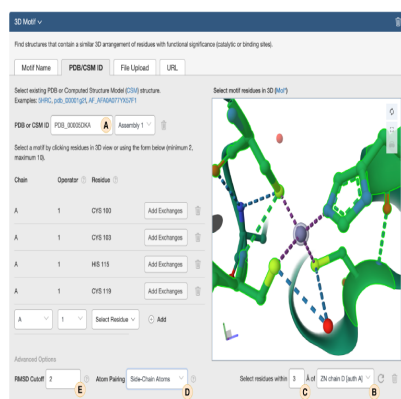




RCSB protein data Bank: Next-generation advances search for exploration of experimental structures and computed structure models

Description

The Protein Data Bank (PDB), established in 1971, is the primary global, open-access archive for experimentally determined 3D macromolecular structures (proteins, RNA, DNA). The research-focused RCSB.org webportal provides access to these data alongside more than one million machine-learning-predicted structure models, greatly expanding the available structural landscape. Rapid growth of both experimental and computational structures has increased the need for powerful yet accessible search tools that serve a broad and diverse scientific community.

Unified Query Builder: Seamlessly combines annotation filters, sequence similarity search and 3D shape similarity into complex Boolean queries.

Integrated 3D Viewer: Features an embedded Mol* 3D tool inside the query builder, allowing you to define structural spatial parameters without needing formal nomenclature or residue numbers

Curated Biological Knowledge: Builds geometry-driven queries using active-site templates from the Mechanism and Catalytic Site Atlas (M-CSA) and ligand-guided structural motifs.

Advanced Chemical Search: Features an integrated chemical drawing tool to query small molecules via standard identifiers (SMILES, InChI, Chemical Formula), linked directly to structural annotations

Cross-Model Exploration: Allows users to query purely experimental data, include AI/ML models (AlphaFold DB and ModelArchive), or isolate **Integrative/Hybrid Methods (IHM)** structures.

The update significantly improves how results are refined, organized, and retrieved:

- **Result Clustering:** Results can be automatically grouped into **UniProt Groups**, Sequence Identity clusters, or Deposition Groups to map trends across related structures.
- **MyPDB Integration:** Users can authenticate via Google, Facebook, or ORCID to store search histories, re-run complex workflows, and subscribe to automatic email updates for weekly data releases.

- **Programmatic Support:** Advanced graphical queries built in the user interface can be exported into **REST and GraphQL API queries** via a dedicated interface

3D Motif ▾

Find structures that contain a similar 3D arrangement of residues with functional significance (catalytic or binding sites).

Motif Name
PDB/CSM ID
File Upload
URL

Select existing PDB or Computed Structure Model (CSM) structure.
Examples: 5HRC, pdb_00001g2f, AF_AFA0A077YX57F1

PDB or CSM ID A

Select a motif by clicking residues in 3D view or using the form below (minimum 2, maximum 10).

Chain	Operator ?	Residue ?		
A	1	CYS 100	Add Exchanges	
A	1	CYS 103	Add Exchanges	
A	1	HIS 115	Add Exchanges	
A	1	CYS 119	Add Exchanges	

▾
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Advanced Options

RMSD Cutoff E ? Atom Pairing D ?

Select motif residues in 3D (Mol*)

Select residues within Å of C E

Category

1. News